THE CYANIDES UPDATE FOR HITRAN2024.

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The comprehensive updates of hydrogen cyanide (HCN) and methyl cyanide (CH_3CN) line lists in the HITRAN database address current needs in both atmospheric monitoring and astrophysical research.

In this work, we validated the MOMeNT-90 [a] line list, which was proposed for updating the HCN line list in HITRAN. This line list utilizes a new, highly accurate potential energy surface (PES) and an ab initio dipole moment surface (DMS). It combines line intensities calculated through variational methods with line centers derived from experimental energy levels, where possible. Furthermore, the list includes broadening parameters. Extensive validations against experimental cross-sections were carried out, and further semi-empirical improvements have been introduced.

Regarding CH_3CN, line parameters were initially included in HITRAN2008, with no updates since then. The predictions were based on a combined fit of rotational and ro-vibrational data involving states up to $v_8 = 2$, which were published by Müller [b]. The analysis took into account interactions between these states as well as interactions of $v_8 = 2$ with $v_4 = 1$, $v_7 = 1$, $v_8 = 3$ and the last three states with each other. This project constructs all available CH_3CN data into a HITRAN-formatted line list, validating it against existing measurements and calculations. The new update is based on a more recent study[c] which includes accurate rotational and rovibrational data of $v_4 = 1$, its associated ν_8 hot band, and slight extensions of the lower state data.

To complement the updates to HCN and CH_3CN line lists in the HITRAN database[d], a brief update to the software tool for calculating look-up tables of cross-sections of different molecules within the HITRAN database under a custom set of pressures, temperatures and volume mixing ratios – X-MASS – will be presented.

[a] Mellau, G. C., *et al.* JQSRT, 270, 107666, 2021.
[b] Müller, H. S., *et al.* JMS, 312, 22-37, 2015.
[c] Müller, H. S., *et al.* JMS, 378, 111449, 2021.
[d] Gordon, I. E., *et al.* JQSRT, 277, 107949, 2021.